Metal-Insulator Transition in Two Dimensions in a Nearly Periodic Potential

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A two-dimensional gas of non-interacting quasiparticles in a nearly periodic potential is considered at zero temperature. The potential is a superposition of a periodic potential, induced by the charge density wave of a Wigner crystal, and a weak random potential due to disorder. There is a metal-insulator transition that is controlled by the strength of the periodic potential. The transition is continuous in the presence of randomness. We evaluate the density of states, which is non-zero at the Fermi energy in the metallic phase, and the dc conductivity. The latter changes with decreasing modulation of the periodic potential from 0 to $\sigma \approx 2e^2/h$.

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The metal-insulator transition in silicon MOSFETs [1] and GaAs/AlAs heterostructures [2] presents a new, unexpected and interesting phenomenon in a two-dimensional electron (or hole) gas [1]. One of the characteristic features of the transition is the scaling behavior of the resistivity with temperature. There is a critical resistivity which shows up at the transition point from the insulating to the conducting regime. The corresponding critical conductivity typically ranges from $0.3e^2/h$ [1] to $2e^2/h$ [2]. In other words, it seems from the experiments that at zero temperature there is either an insulating state or a conducting state with a conductivity equal or larger than a critical (minimal) conductivity. The nature of the conducting state (high electron density) is unclear. It is either a normal metal [3], a superconducting state [4] or a state controlled by charged traps [5]. The nature of the insulating state (low electron density), on the other hand, is less controversal. Since the 2D electron gas must have a high mobility in order to undergo a transition to a non-insulating state, disorder is very weak in the samples. Therefore, a Wigner crystal or at least a modulated electron density with short range order is expected due to the Coulomb interaction [6]. In the following we shall discuss a model which provides a simple picture of a metal-insulator transition in a nearly periodic potential created by a modulated electron density. The discussion will focus on the approach of the conducting regime, coming from the insulating regime, but does not include a description of this regime away from the transition point.

Lattice dynamics calculations [7,8] and computer simulations [9,10] for the pure 2D electron gas indicate that the Wigner crystal forms a hexagonal lattice. Quasiparticles, which are the excitations in the Wigner crystal, experience an effective potential due to the modulation of the electron density. Formally, the dynamics of the quasiparticles can be derived from the model of a 2D electron gas which is subject to Coulomb interaction. Starting with a microscopic model we can apply a self-consistent approximation for the space-dependent electron density n (cf. [11]), which describes the Wigner crystal, and regard the fluctuations around the static electron density as quasiparticles. In leading order the interaction of the fluctuations is neglected, i.e. we consider independent quasiparticles. This approach is analogous to the derivation of the Bogoliubov de Gennes Hamiltonian in a superconductor, where the superconducting order parameter Δ is treated in a self-consistent (BCS) approximation. In contrast to Δ the electron density n couples directly to the quasiparticle density. Therefore, it can be considered as an effective potential for the quasiparticles. The latter prefer to stay in places with low electron density (minimal potential, the circles shown in Fig. 1.) but can also tunnel through the saddle points of the potential between these potential minima (dashed lines in Fig. 1).

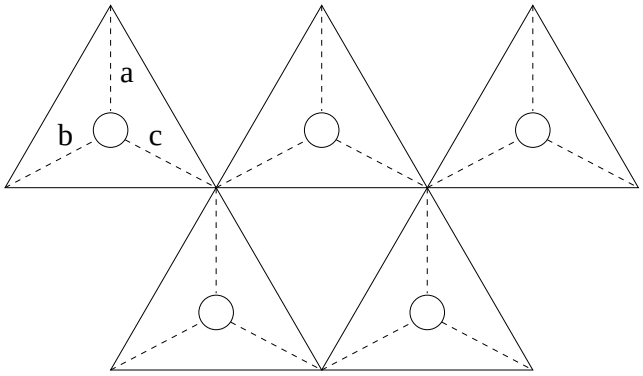

FIG. 1. Effective potential and the lattice of the tight-binding model. Circles indicate minima of the electron density and dashed lines the tunneling of the quasiparticles.

The model of the quasiparticles can be further simplified by assuming a discrete potential instead of the smoothly varying density n. In other words, the variation of n is taken into account only down to a finite length scale. For the latter we choose the distance between a minimum and an adjacent saddle point. This is a minimal model in order to study the broken translational invariance caused by the density modulation. It can be considered as a tight-binding approximation for the quasiparticles, where the lattice points are the minima and the saddle points of the electron density. There is a potential $V_{\mathbf{R}}$ at each lattice site $\mathbf{R}$ with $V_{\mathbf{R}} = V_+$ on the minima and $V_{\mathbf{R}} = V_-$ on the saddle points. For

the sake of simplicity of our model, (I) only the overlap between nearest neighboring lattice sites (i.e. a minimum and a saddle point) and (II) no spin effect are taken into account. It is convenient to substract a constant potential in order to replace $V_{\mathbf{R}}$ by the modulation $m_{\mathbf{R}} \equiv V_{\mathbf{R}} - (V_+ + V_-)/2$. Then $m_{\mathbf{R}}$ is a staggered field on the lattice with $m_{\mathbf{R}} = \pm(V_+ - V_-)/2 \equiv \pm m$. This field breaks the translational invariance on the lattice. A translational-invariant representation can be obtained from one of the two sublattices. Using the sublattice of the maxima (circles in Fig. 1), the co-ordinates of a site on this sublattice are $\mathbf{r} = (x, y)$, where the x (y) direction is horizontal (vertical) in Fig. 1. The co-ordinates of a site of the other sublattice (corners of the triangles in Fig. 1) are obtained by shifting the co-ordinates $\mathbf{r}$ with the unit vector $\mathbf{a} = (0, 1)$. Any site $\mathbf{R}$ on the lattice can now be written as $(\mathbf{r}, j) \equiv \mathbf{r} + (j-1)\mathbf{a}$, where $j = 1, 2$ is the index of the sublattice.

The quasiparticle Hamiltonian is defined as

$$\hat{H} = \sum_{\mathbf{r},\mathbf{r}'} \sum_{j,j'=1}^{2} H_{\mathbf{r},j;\mathbf{r}',j'} c^{\dagger}_{\mathbf{r},j} c_{\mathbf{r}',j'}, \tag{1}$$

where c ($c^{\dagger}$) are the annihilation (creation) operators of the (fermionic) quasiparticles. For the off-diagonal matrix elements we assume $H_{\mathbf{r},\mathbf{r}+\mathbf{e}} = t$, where the unit vectors $\mathbf{e} = \mathbf{a}, \mathbf{b}, \mathbf{c}$ are indicated in Fig. 1. This Hamiltonian has also been studied in connection with the quantum Hall effect. [12] The matrix $H = H_0 + m\sigma_3$, where the Pauli matrix σ_3 refers to the sublattice index, can be given in Fourier representation with respect to the sublattices ($\mathbf{r} \to (k_x, k_y)$) as

$$H \to \tilde{H} = t[c(k_x, k_y)\sigma_1 + s(k_x, k_y)\sigma_2] + m\sigma_3 \tag{2}$$

with Pauli matrices σ_1, σ_2 and

$$c(k_x, k_y) = \cos(-k_y) + \cos(\sqrt{3}k_x/2 + k_y/2) + \cos(-\sqrt{3}k_x/2 + k_y/2). \tag{3}$$

$s(k_x, k_y)$ is obtained from this expression by replacing the cosine by sine. For this translational-invariant Hamiltonian we obtain the dispersion

$$E_{\pm}(k_x, k_y) = \pm\sqrt{m^2 + t^2(c^2 + s^2)} \tag{4}$$

as shown in Fig. 2. The modulation m creates a gap between the two bands with $E_+ > 0$ and with $E_- < 0$. This gap vanishes only in the limit of a vanishing modulation $m = 0$. Thus our system is insulating as long as we have a modulated electron density. In the case $m = 0$ there are six nodes (k_x, k_y) on a circle with radius $4 \cdot 3^{-3/2}\pi$, located at

$$(\pm\frac{4\pi}{3^{3/2}}, 0), \quad (\frac{2\pi}{3^{3/2}}, \pm\frac{2\pi}{3}), \quad (-\frac{2\pi}{3^{3/2}}, \pm\frac{2\pi}{3}). \tag{5}$$

For the analysis of the transport (i.e. low energy) properties of this system it is sufficient to study the properties associated with the nodes. Expansion around the two nodes at $(\pm 4\pi/3^{3/2}, 0)$ leads to the Dirac Hamiltonians

$$H_0 \sim \pm(3t/2)(k_1\sigma_1 \pm k_2\sigma_2), \tag{6}$$

and around the other four nodes to

$$H_0 \sim -(3t/4)[(\sqrt{3}k_1 + k_2)\sigma_1 + (\sqrt{3}k_1 - k_2)\sigma_2], \tag{7}$$

where k_1 (k_2) is now the deviation from the corresponding node in x- (y-) direction. Thus for the pure system the Hamiltonian separates into the six nodes when we consider small energy (i.e. large scale) behavior, where the vicinity of each node is given by a two-dimensional Dirac operator.

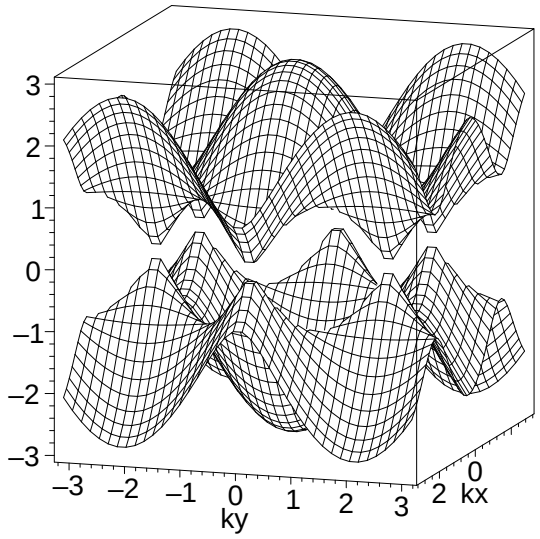

FIG. 2. Dispersion $E(k_x, k_y)$ of quasiparticles, measured in units of the overlap t.

So far we have assumed that there is perfect long-range order in the Wigner crystal, leading to a translational-invariant Hamiltonian for the quasiparticles. This is an idealization which is not valid in a real system where we have always impurities. It is known that the 2D Wigner crystal can be strongly affected by impurities. In the presence of a high density of impurities the crystalline order is destroyed completely and an electron glass can be created [13]. On the other hand, short-range order may survive if disorder is only weak. This situation can be described in terms of the quasiparticles by a weak random perturbation added to the periodic modulation. Various types of disorder are possible but we will restrict the discussion to the simplest case,

$$M_{\mathbf{r}}\sigma_3 = (m + \delta M_{\mathbf{r}})\sigma_3, \tag{8}$$

assuming that the effect of this type of randomness describes a generic situation.

In principle, the disorder δM can couple different nodes because the random term has fluctuations on all length scales. However, we will assume that the overlap

between the scales, related to the various nodes, is negligible, i.e. for k and k' belonging to the vicinities of two different nodes we have

$$\sum_{\mathbf{r}} e^{-i\mathbf{k}\cdot\mathbf{r}+i\mathbf{k}'\cdot\mathbf{r}} M_{\mathbf{r}} \approx 0. \tag{9}$$

For each node we introduce an independent random term $\delta M_{\alpha,\mathbf{r}}$ which means that $M_{\alpha,\mathbf{r}}$ fluctuates only on scales which are compatibel with the corresponding node. We assume a Gaussian distribution with $\langle \delta M_{\alpha,\mathbf{r}} \rangle = 0$ and $\langle \delta M_{\alpha,\mathbf{r}} \delta M_{\alpha',\mathbf{r}'} \rangle = g\delta_{\alpha,\alpha'}\delta_{\mathbf{r},\mathbf{r}'}$. Then the Green's function $G(z) = (H-z)^{-1}$ can be block-diagonalized with respect to the six nodes as diag$[(H_1 - z)^{-1}, ..., (H_6 - z)^{-1}]$ with independent Dirac Hamiltonians

$$H_\alpha = i(a_\alpha \nabla_1 + b_\alpha \nabla_2)\sigma_1 + i(c_\alpha \nabla_1 + d_\alpha \nabla_2)\sigma_2 + M_{\alpha,\mathbf{r}}\sigma_3, \tag{10}$$

where $a_\alpha = -d_\alpha = -3t/2$, $b_\alpha = c_\alpha = 0$ for the nodes with $k_y = 0$ (i.e. $\alpha = 1, 2$) and $a_\alpha = c_\alpha = -3^{3/2}t/4$, $b_\alpha = -d_\alpha = -3t/4$ for the nodes with $k_y \neq 0$ (i.e. $\alpha = 3, ..., 6$). The block-diagonal structure is a crucial simplification because we only have to evaluate the physical quantities for the six nodes independently. The density of states (DOS) and the conductivity of the corresponding Dirac Hamiltonians are known and shall be discussed subsequently.

The DOS of a system near a metal-insulator transition exhibits a characteristic behavior. In the simplest case there is a gap in the insulating phase which closes at the transition to the metal. The closing of the gap was measured recently in a tunneling experiment near the metal-insulator transition of boron-doped silicon crystals, a three-dimensional electron gas. [14] It was found that the DOS goes roughly like a power law $\rho(E) \sim \rho_0(|E|/E_0)^\gamma$ (E is the distance from the Fermi energy E_F and $\gamma \approx 0.5$) in the insulating phase and like $\rho(E) \sim \rho_0[1 + (|E|/E_0)^\gamma]$ in the metallic phase. Thus the insulating phase can be distinguished from the metallic phase only for energies close to the Fermi energy. A similar behavior is expected for a two-dimensional system, with a different exponent γ though. For instance, a linear behavior $\rho(E) \sim \rho_0|E|/E_0$ was observed in a 2D electron gas subject to a perpendicular magnetic field. [15] This result is in agreement with the effective Dirac fermion description of quasiparticles in a quantum Hall system [12] which also gives a linear DOS in the absence of disorder. Moreover, a linear behavior of the DOS was found in a mean-field calculation of a disordered 2D electron gas. [13]

In our model, the block-diagonal structure enables us to write the DOS as a sum of DOS's of the vicinity of each node. Using the result of the Dirac fermions from a saddle point approximation this gives for $m = 0$ at each node α [16]

$$\rho_\alpha(E) \approx \frac{e^{-\pi/g}}{g} + |E|^\gamma, \tag{11}$$

where the exponent γ varies with increasing randomness g from 1 to 0 (Fig. 3).

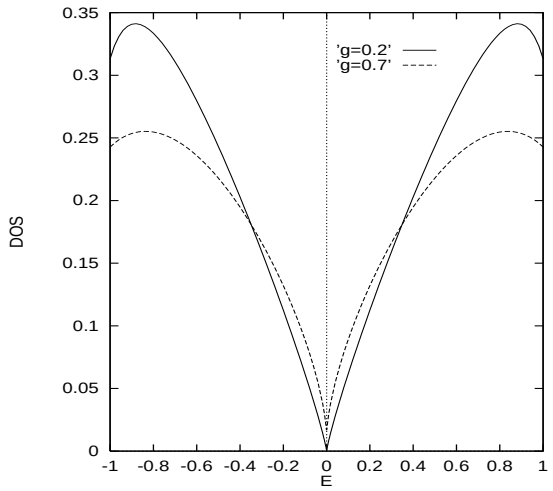

FIG. 3. Density of states at $m = 0$ for different strength of randomness

The energy scale is set by the overlap t. The DOS as a function of the modulation parameter m at $E = 0$ is $\propto \sqrt{4e^{-2\pi/g} - m^2}\Theta(4e^{-2\pi/g} - m^2)/2g$. Therefore, the DOS vanishes with $g \to 0$. The effect of the periodic modulation is the creation of a gap. On the other hand, the random fluctuations around the periodic modulation create states at the Fermi energy as long as the random fluctuations are strong relative to the periodic modulation. To have quasiparticle states at the Fermi energy it requires random fluctuations, characterized by the parameter $2e^{-\pi/g}$, which are larger than the periodic modulation, characterized by m, . The creation of new states around $m = 0$ by the randomness can be explained by the formation of tail states at low energy. This is similar to the creation of Lifshitz tails. [20] However, it will be discussed in the following that these states are conducting - in contrast to the localized states in the Lifshitz tails.

In the presence of a gap the conductivity vanishes with vanishing temperature. Here we are only interested in zero temperature properties, i.e. we must study the transport properties for the system with a closed gap. Since a randomly disturbed modulation ($\delta M_r \neq 0$) creates states at the Fermi level for $m \leq 2e^{-\pi/g}$, the case of the nearly periodic modulation is a candidate for a metal-insulator transition. However, the vanishing gap is necessary but not sufficient for a conducting state because the quasiparticle states might be localized by randomness. The localization effect is known to be very efficient in $d = 2$, e.g., all quantum states are localized according to conventional scaling theory for localization [17]. How-

ever, it was found that Dirac fermions with random mass can escape from localization by a special mechanism due to symmetry breaking [18]. It leads to diffusion of the Dirac particle for sufficiently small average mass, i.e. for sufficiently small modulation. The conductivity can be evaluated using the Kubo-Greenwood formula. Then the dc conductivity at $T = 0$ and $E = 0$ reads

$$\sigma \approx \frac{e^2}{h} \lim_{\eta \to 0} \eta^2 \sum_{\mathbf{r}} \mathbf{r}^2 \mathrm{Tr}_2 \langle G(0, \mathbf{r}; i\eta) G(\mathbf{r}, 0; -i\eta) \rangle$$
$$= -\frac{e^2}{h} \lim_{\eta \to 0} \eta^2 \nabla_k^2 \tilde{C}(k, \eta)|_{k=0} \qquad (12)$$

with the two-particle Green's function $C(\mathbf{r}, \eta) = \mathrm{Tr}_2 \langle G(0, \mathbf{r}; i\eta) G(\mathbf{r}, 0; -i\eta) \rangle$. The latter is a sum of contributions from the six different nodes due to the block-diagonal form of the single-particle Green's function. The average two-particle Green's function can be diagonalized by a Fourier transformation because it is translational invariant as a consequence of the uniform distribution of the randomness. The nodes require a similarity transformation

$$k_1 \to k_1' = a_\alpha k_1 + b_\alpha k_2, \quad k_2 \to k_2' = c_\alpha k_1 + d_\alpha k_2 \qquad (13)$$

in order to obtain the usual Dirac form $\sigma \cdot k$ for the Hamiltonian. The average two-particle Green's function is [18]

$$\tilde{C}_\alpha(k, \eta) = \frac{\pi}{2} \frac{\rho}{\eta + D({k_1'}^2 + {k_2'}^2)/|a_\alpha d_\alpha - b_\alpha c_\alpha|}, \qquad (14)$$

where D is the diffusion coefficient of the Dirac fermions. The extra factor $1/|a_\alpha b_\alpha - c_\alpha d_\alpha|$ is the Jacobian of the transformation $k \to k'$. For weak disorder ($g \ll 1$) the diffusion coefficient is [19]

$$D \approx \frac{1}{2\pi^2 \rho} (1 - x^2)[1 - \frac{g}{2\pi}(1 - 2x^2)] \Theta(1 - x^2) \qquad (15)$$

with $x = me^{\pi/g}/2$. With (12) and the summation over all nodes this implies for the conductivity

$$\sigma(m) \approx \frac{e^2}{h} s_0 (1 - x^2)[1 - \frac{g}{2\pi}(1 - 2x^2)] \Theta(1 - x^2) \qquad (16)$$

with $s_0 \approx 2.1$. The conductivity depends on the modulation m which scales with $e^{\pi/g}$. The transition is very sharp for weak disorder, since the scale is exponential, and it is discontinuous with a minimal conductivity $2e^2/h$ if disorder is absent.

The quasiparticle states overlap in such a manner that they form conducting states. This effect is known for Dirac fermions with randomness already in one dimension, where the zero energy modes are extended. [20] However, in contrast to the finite diffusion coefficient (15), leading to a diffusive behavior of quasiparticles, this coefficient is singular then. In our model the diffusion is valid only for weak randomness, as it is indicated by the vanishing diffusion coefficient (15) if $g = 2\pi$.

In conclusion, a possible metallic state in a two-dimensional electron gas is approached from an insulating regime by the destruction of the gap of the insulating state by disorder. Our discussion is based on a simple model for quasiparticles in a nearly periodically modulated electron density, which can be considered as a Wigner solid with weak disorder. The system becomes metallic for a sufficiently weak modulation with a conductivity $\sigma \approx 2e^2/h$. The latter decreases linearly with increasing disorder. The conductivity varies continuously for the nearly periodic potential.

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[1] S.V. Kravchenko et al., Phys. Rev. B **50**, 8039 (1994); S.V. Kravchenko et al., Phys. Rev. Lett. **77**, 4938 (1996).
[2] M.Y. Simmons et al., Phys. Rev. Lett. **80**, 1292 (1998).
[3] C. Castellani, C. Di Castro and P.A. Lee, Phys. Rev. B **57**, R9381 (1998).
[4] D. Belitz and T.R. Kirkpatrick, Phys. Rev. B **58**, 8214 (1998).
[5] B.L. Altshuler and D.L. Maslov, Phys. Rev. Lett. **82**, 145 (1999).
[6] Jongsoo Yoon et al., Phys. Rev. Lett. **82**, 1744 (1999).
[7] G. Meissner et al., Phys. Rev. B **13**, 1370 (1976).
[8] L. Bonsall and A.A. Maradudin, Phys. Rev. B **13**, 1959 (1976).
[9] D. Ceperley, Phys. Rev. B **18**, 3126 (1978).
[10] B. Tanatar and D.M. Ceperley, Phys. Rev. B **39**, 5005 (1989).
[11] E. Fradkin: *Field Theories of Condensed Matter Systems*, (Addison - Wesley, Redwood City, 1991).
[12] G.W. Semenoff, Phys. Rev. Lett. **53**, 2449 (1984) ; F.D.M. Haldane, Phys. Rev. Lett. **61**, 2015 (1988).
[13] A.A. Pastor and V. Dobrosavlević, Phys. Rev. Lett. **83**, 4642 (1999)
[14] M. Lee et al., Phys. Rev. B **60**, 1582 (1999)
[15] H.B. Chan et al., Phys. Rev. Lett. **79**, 2867 (1997).
[16] U. Eckern and K. Ziegler, J. Phys. Condens. Matter **10**, 6749 (1998).
[17] E. Abrahams et al., Phys. Rev. Lett. **42**, 673 (1979).
[18] K. Ziegler, Phys. Rev. B **55**, 10661 (1997), Phys. Rev. Lett. **80**, 3113 (1998).
[19] G. Jug and K. Ziegler, Phys. Rev. B **59**, 5738 (1999).
[20] I.M. Lifshits, S.A. Gredeskul, and L.A. Pastur, *Introduction to the Theory of Disordered Systems* (Wiley, New York, 1988).